Succinic acid, 2,3-dichlorophenyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C12H9Cl5O4/c13-7-2-1-3-8(11(7)14)21-10(19)5-4-9(18)20-6-12(15,16)17/h1-3

InchiKey: LUBQMYKLFGLTTI-UHFFFAOYSA-N

Formula: C12H9Cl5O4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1Cl)OCC(Cl)(Cl)Cl

Mol. weight [g/mol]: 394.46

Physical Properties

Property code	Value	Unit	Source
gf	-381.34	kJ/mol	Joback Method
hf	-654.47	kJ/mol	Joback Method
hfus	39.24	kJ/mol	Joback Method
hvap	84.85	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.592		Crippen Method
mcvol	232.260	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	2481.00		NIST Webbook
rinpol	2481.00		NIST Webbook
tb	847.10	K	Joback Method
tc	1084.78	K	Joback Method
tf	572.80	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.31	J/mol×K	847.10	Joback Method
cpg	553.38	J/mol×K	886.71	Joback Method
cpg	560.56	J/mol×K	926.33	Joback Method
cpg	566.89	J/mol×K	965.94	Joback Method
cpg	572.40	J/mol×K	1005.55	Joback Method
cpg	577.12	J/mol×K	1045.17	Joback Method
cpg	581.10	J/mol×K	1084.78	Joback Method
dvisc	0.0003971	Pa×s	572.80	Joback Method

dvisc	0.0002626	Pa×s	618.52	Joback Method
dvisc	0.0001838	Pa×s	664.23	Joback Method
dvisc	0.0001347	Pa×s	709.95	Joback Method
dvisc	0.0001025	Pa×s	755.67	Joback Method
dvisc	0.0000805	Pa×s	801.38	Joback Method
dvisc	0.0000649	Pa×s	847.10	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390242&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume